Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Chiroptical, Linear, and Quadratic Nonlinear Optical Properties of the Tetrathiafulvalenylallene: Multifunctional Molecular Material

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Table S1. The calculated bond length (in Å) in both neutral state and the cation states and the BLA values.

	1	$\mathbf{1}^{2+}$	$\mathbf{1}^{4+}$
r_a	1.349	1.387	1.420
$r_{a'}$	1.348	1.358	1.368
$r_{a''}$	1.354	1.375	1.421
r_b	1.781	1.758	1.726
r_c	1.783	1.783	1.735
r_d	1.787	1.762	1.734
r_e	1.781	1.753	1.741
$r_{b'}$	1.781	1.756	1.731
$r_{c'}$	1.785	1.752	1.738
$r_{d'}$	1.786	1.772	1.717
$r_{e'}$	1.753	1.731	1.766
Δr	0.429	0.385	0.333

Note: $r_{a'}$ is close to the center of the centroid, but $r_{a''}$ is far away of the centroid.

Table S2 The calculated dipole moment (μ, Debye) of the studied compound in neutral and cationic states.

	μ
1	4.67
$\mathbf{1}^{2+}$	6.58
$\mathbf{1}^{4+}$	7.27

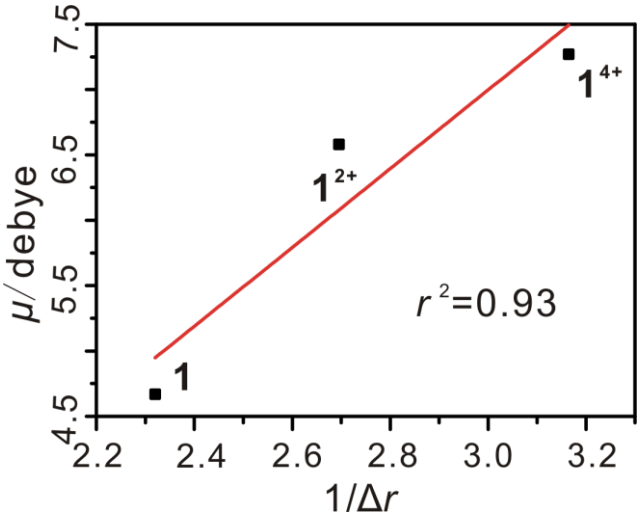


Figure S1 Dependence of the dipole moment on the inverse of the BLA value (Δ*r*).

Table S3. Computed absorption energy (nm) and oscillators strengths (*f*) using B3LYP functional at different basis sets level for compound **1**

Basis set	absorption	*f*	absorption	*f*
6-31G(d,p)	386.3	0.082	282.5	0.229
6-31G+(d)	394.4	0.082	287.9	0.177
6-311G(d,p)	394.8	0.087	285.8	0.144
6-31G++(d,p)	395.2	0.079	287.2	0.147
6-311G++(d,p)	397.5	0.077	288.3	0.127
6-311G++(2d,2p)	404.5	0.084	275.8	0.137
Experiment	404		260	

Table S4. Computed absorption energy (nm) and oscillators strengths (*f*) using different functionals at 6-311++G(2d,2p) basis set level for compound **1**

Functionals	absorption	*f*	absorption	*f*
CAM-B3LYP	404.8	0.022	269.6	0.226
M05-2X	423.3	0.018	278.2	0.376
BH&HLYP	390.6	0.027	265.2	0.447

PBE0	408.0	0.018	266.7	0.222
B3LYP	404.5	0.084	275.8	0.137
Exp	404		260	

Here, we selected six Pople's basis sets: 6-31G(d,p), 6-31G+(d), 6-311G(d,p), 6-31G++(d,p), 6-311G++(d,p) and 6-311++G(2d,2p) to evaluate the effect of the basis set extension on the properties of electron transition by using B3LYP functional. It is noted that compound **1** exhibits an intense absorption band at 260 nm and a moderately intense absorption band at 404 nm measured by Hasegawa et al.[18] The calculated results at the different basis sets level were listed in Table 1. On this table, the calculated absorption wavelengths become much closer to the experimental ones with increasing the basis set size. Moreover, the relative strength of the two absorption bands are reproduced by the selected basis sets. Jacquemin and Adamo found that diffuse functions are necessary to obtain correct vertical transition energies and 6-311++G(2d,2p) basis set give the best results for their studied compounds.[1] Thus, 6-311++G(2d,2p) basis set was used in the following calculation. Likewise, five DFT functionals: CAM-B3LYP,[2] M05-2X,[3] BH&HLYP,[4] PBE0,[5] and B3LYP,[6] were selected to assess the effect of DFT functionals on the computed properties. These functionals have exhibited good performance in predicting the electron transition for organic compounds. In Table 2, we listed the absorption energy and oscillators strengths of these functionals. It is interesting to find that the absorption energy data computed with CAM-B3LYP, PBE0, and B3LYP are similar and closer to the experimental ones. However, the performance of M05-2X and BH&HLYP is not good for our studied compound. To further test the performance of CAM-B3LYP,

PBE0, and B3LYP functionals on UV-Vis/CD spectra, their simulated spectra were shown in Figure S3. The spectra simulated by PBE0 and B3LYP are good agreement with the experimental ones and better than these of CAM-B3LYP. B3LYP functional has been widely used to simulate the ECD spectra and assign absolute configurations. So, the results of B3LYP functional combined with 6-311++G(2d,2p) basis set were used in this paper.

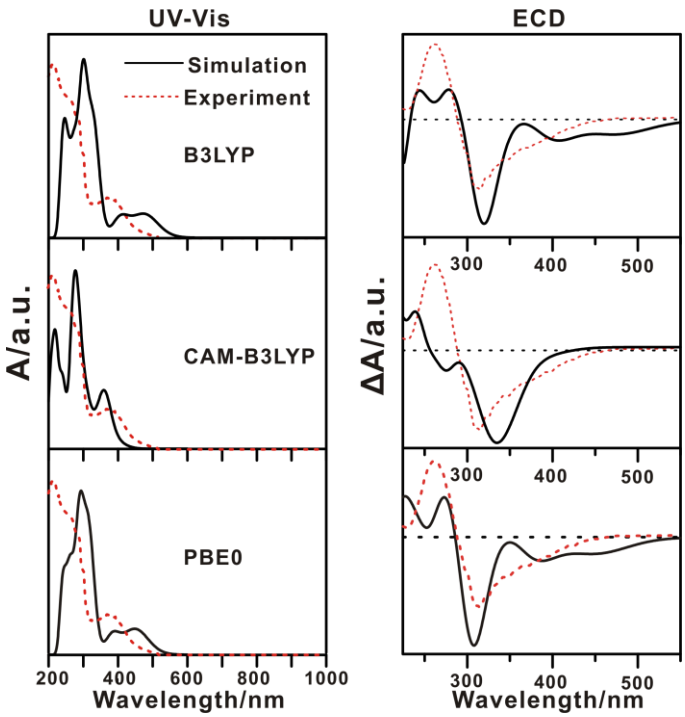


Figure S2. Calculated UV-Vis (left) and ECD (right) spectra of compound **1** using CAM-B3LYP, PBE0, and B3LYP functionals at the 6-311++G(2d,2p) basis set level along with experimental UV-Vis and ECD (red dash line).

Table S5. The Calculated excitation energies, oscillator strengths and rotational strengths for the neutral state in the gas phase at the B3LYP/ 6-311++G(2d,2p) level.

states	eV	λ^a	f^b	Rlength[c]	Rvelocity[c]

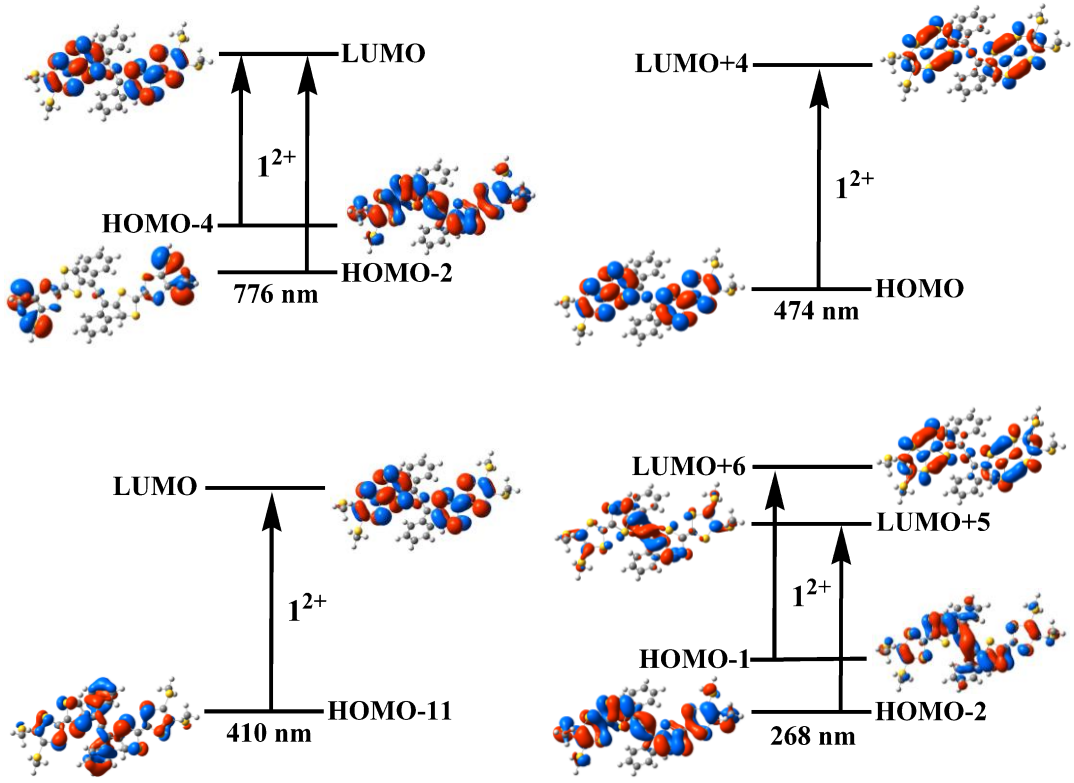
1	2.5484	486.53	0.0139	32.3298	32.9941
2	2.5502	486.17	0.0753	-115.6311	-112.6302
3	2.7311	453.97	0.0428	-12.4941	-14.8339
4	2.7331	453.65	0.0023	-9.6141	-9.1218
5	2.9004	427.47	0.0213	53.3427	51.6782
6	2.9066	426.56	0.0013	-57.1453	-54.5661
7	3.0649	404.53	0.0835	-214.4723	-213.6357
8	3.1175	397.71	0.0130	112.4199	112.8798
9	3.2913	376.71	0.0026	-6.7786	-6.7903
10	3.2954	376.23	0.0012	7.2690	7.3160
11	3.3284	372.50	0.0000	-0.1400	-0.2118
12	3.3293	372.40	0.0026	5.2453	5.1555
13	3.6167	342.81	0.0026	-14.7222	-14.3569
14	3.6233	342.19	0.0147	32.9122	32.9835
15	3.7136	333.86	0.0017	-1.6325	-1.5993
16	3.7198	333.31	0.0126	27.7771	27.4815
17	3.7481	330.79	0.2083	-356.5556	-351.3821
18	3.7553	330.16	0.0189	62.6716	61.7988
19	3.7875	327.35	0.2414	-281.3915	-282.1693
20	3.8021	326.09	0.0005	-0.0666	-0.0646
21	3.8128	325.18	0.0106	9.6694	7.4852
22	3.8297	323.74	0.0043	-2.3073	-2.2479
23	3.8464	322.34	0.0043	11.2466	11.0586
24	3.9521	313.72	0.0855	-8.7510	-9.0745
25	3.9691	312.37	0.0044	15.6280	16.0420
26	3.9859	311.05	0.0051	55.9486	57.5525
27	4.0200	308.42	0.0352	-13.4734	-12.7622
28	4.0345	307.31	0.0300	25.4415	24.3947
29	4.0935	302.88	0.0060	17.0668	16.8096
30	4.0983	302.53	0.0005	0.8876	0.7653
31	4.1570	298.26	0.3653	-443.4723	-439.9209
32	4.1765	296.86	0.1279	268.5751	260.9055
33	4.1908	295.85	0.1525	-126.2728	-123.1978
34	4.2022	295.05	0.0651	341.4947	345.3833
35	4.2152	294.14	0.0008	17.6378	18.9977
36	4.2178	293.95	0.0130	15.2837	15.0379
37	4.2337	292.85	0.0133	22.8241	22.4052
38	4.2354	292.74	0.0026	-33.3136	-29.8663
39	4.2916	288.90	0.0033	-15.0654	-14.4377
40	4.2957	288.63	0.0049	16.8593	16.7948
41	4.3105	287.63	0.0001	-9.2578	-7.9355
42	4.3130	287.47	0.0108	0.7634	0.6906
43	4.3190	287.07	0.0022	24.6816	25.7676
44	4.3210	286.93	0.0131	-6.6289	-6.2168

45	4.3965	282.01	0.0010	-7.8192	-8.6027
46	4.3992	281.83	0.0007	1.4419	1.2067
47	4.4107	281.10	0.0001	-0.8913	-0.8975
48	4.4123	281.00	0.0130	-9.5732	-9.2469
49	4.4571	278.17	0.0004	4.2033	3.6382
50	4.4637	277.76	0.0633	-13.2166	-13.4163
51	4.4957	275.78	0.1366	-0.9120	-2.1400
52	4.5044	275.25	0.0012	-7.2594	-7.1635
53	4.5052	275.20	0.0005	-1.0440	-0.9676
54	4.5172	274.47	0.0002	11.0767	11.3798
55	4.5211	274.23	0.0794	43.5167	43.4467
56	4.5549	272.20	0.0035	-37.3395	-36.5207
57	4.5718	271.19	0.0059	11.3717	11.4861
58	4.5863	270.33	0.0037	-25.8026	-26.6156
59	4.5908	270.07	0.0248	32.7708	32.7283
60	4.6034	269.33	0.0141	-41.2473	-41.3448
61	4.6129	268.78	0.0082	14.2644	12.8434
62	4.6363	267.42	0.0001	-4.9367	-4.4035
63	4.6585	266.15	0.0329	18.7699	18.0519
64	4.6598	266.07	0.0005	-21.4681	-17.8002
65	4.6680	265.60	0.0002	9.0384	5.6317
66	4.6798	264.93	0.1240	66.8543	66.7812
67	4.7239	262.46	0.0026	12.6978	11.3831
68	4.7265	262.31	0.0025	4.1424	4.1890
69	4.7331	261.95	0.0006	1.3590	1.1779
70	4.7370	261.74	0.0001	-9.2721	-7.7956
71	4.7656	260.17	0.0236	-8.5130	-8.4079
72	4.7677	260.05	0.0001	2.7839	3.3347
73	4.7686	260.00	0.0023	0.7858	0.6388
74	4.7812	259.32	0.0143	-32.4935	-32.5281
75	4.7822	259.26	0.0024	36.1130	30.2876
76	4.7894	258.87	0.0000	-0.0993	0.7486
77	4.7962	258.50	0.0040	-20.5288	-20.4824
78	4.8100	257.76	0.0005	12.3135	13.1911
79	4.8372	256.32	0.0113	22.8298	22.3772
80	4.8608	255.07	0.0140	40.7280	40.5576
81	4.8646	254.87	0.0178	-55.3431	-52.8228
82	4.8687	254.66	0.0064	-30.0589	-31.2185
83	4.8712	254.53	0.0076	18.7462	18.5381
84	4.8850	253.81	0.0068	-5.4186	-5.2514
85	4.8939	253.34	0.0049	-11.4086	-10.7786
86	4.9006	253.00	0.0208	-2.5864	-2.6696
87	4.9022	252.92	0.0183	14.5977	14.6074
88	4.9273	251.63	0.0805	45.8110	46.4261

89	4.9615	249.89	0.0159	-29.7517	-29.4794
90	4.9706	249.44	0.0055	-3.0359	-3.3126
91	4.9746	249.23	0.0299	85.7216	81.0855
92	4.9912	248.41	0.0150	0.8710	0.8917
93	4.9947	248.23	0.0005	-6.1979	-4.9227
94	4.9984	248.05	0.0049	27.4791	27.7791
95	5.0019	247.87	0.0047	-2.0222	-2.5757
96	5.0213	246.92	0.0072	31.5876	31.2333
97	5.0224	246.86	0.0001	-4.5812	-3.7348
98	5.0227	246.85	0.0003	1.0608	1.1087
99	5.0308	246.45	0.0024	-11.5192	-11.1395
100	5.0310	246.44	0.0037	14.2987	13.6141
101	5.0325	246.36	0.0000	1.4602	1.4725
102	5.0504	245.49	0.0060	-11.5183	-11.8582
103	5.0635	244.86	0.0358	15.7748	15.7230
104	5.0777	244.18	0.0585	3.3649	3.4726
105	5.0794	244.09	0.0007	-8.5727	-8.8885
106	5.1023	243.00	0.0157	24.1988	24.3356
107	5.1037	242.93	0.0019	27.4478	28.0605
108	5.1131	242.48	0.0004	0.6177	0.6721
109	5.1135	242.46	0.0125	-50.2283	-48.1091
110	5.1180	242.25	0.0064	-29.8715	-30.5754
111	5.1472	240.88	0.0055	17.2787	17.2086
112	5.1474	240.87	0.0467	11.1596	10.9485
113	5.1494	240.78	0.0033	-1.3696	-1.3785
114	5.1564	240.45	0.0181	13.2677	13.4334
115	5.1583	240.36	0.0320	-73.1446	-72.9510
116	5.1669	239.96	0.0346	-25.5944	-25.2737
117	5.1786	239.42	0.0139	-24.5834	-24.8973
118	5.1849	239.13	0.0347	-35.0354	-35.7156
119	5.1918	238.81	0.0003	4.1806	4.0794
120	5.1929	238.76	0.0110	-3.3800	-3.5369
121	5.2069	238.12	0.0103	-70.8779	-71.3095
122	5.2073	238.10	0.0080	0.9910	0.7825
123	5.2141	237.78	0.0013	-10.8294	-9.7935
124	5.2162	237.69	0.0339	25.6424	24.9982
125	5.2396	236.63	0.0032	3.2572	3.9148
126	5.2432	236.47	0.0079	-16.5958	-14.5375
127	5.2587	235.77	0.0073	7.0394	7.1914
128	5.2704	235.25	0.0199	37.0927	37.3277
129	5.2787	234.88	0.0067	9.3691	9.5280
130	5.2847	234.61	0.0306	-30.2070	-30.0283
131	5.2898	234.39	0.0061	-14.0198	-14.0938
132	5.3048	233.72	0.0000	-0.4194	-0.3758

133	5.3069	233.63	0.0064	-15.1962	-14.7754
134	5.3095	233.51	0.0003	2.4339	3.4482
135	5.3137	233.33	0.0056	-10.7881	-10.6136
136	5.3193	233.09	0.0006	2.3218	2.0097
137	5.3233	232.91	0.0005	-1.2466	-1.6328
138	5.3249	232.84	0.0055	1.4243	1.4699
139	5.3385	232.25	0.0003	-0.3726	-0.4291
140	5.3415	232.11	0.0157	-32.8992	-33.7209
141	5.3474	231.86	0.0066	8.6208	8.5773
142	5.3514	231.68	0.0216	-12.1307	-12.0073
143	5.3610	231.27	0.0038	3.5764	3.8452
144	5.3611	231.27	0.0004	2.4638	2.8351
145	5.3654	231.08	0.0018	8.0943	8.0957
146	5.3843	230.27	0.0106	42.2503	42.8001
147	5.3977	229.70	0.0149	-15.5287	-15.0056
148	5.4009	229.56	0.0033	12.8083	13.0162
149	5.4127	229.06	0.0003	-3.8770	-4.4252
150	5.4148	228.97	0.0254	-25.0266	-24.6692

[a] λ in nm. [b] Oscillator Strengths. [c] R values (in 10^{-40} esu^2cm^2) using the velocity-gauge representation and length-gauge representation of the electric dipole operator.



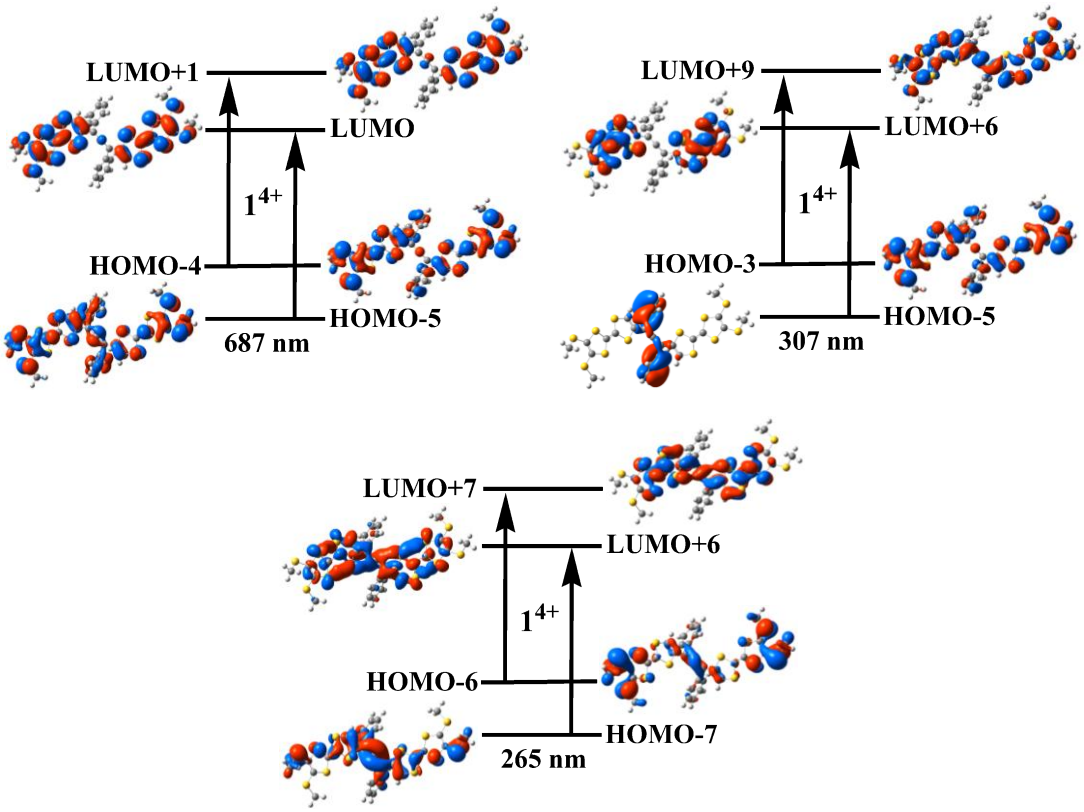


Figure S3. Molecular orbital isosurfaces involved in the main electron transitions of the cationic states $\mathbf{1}^{2+}$ and $\mathbf{1}^{4+}$ at the TDB3LYP/6-311++G(2d,2p) level of theory.

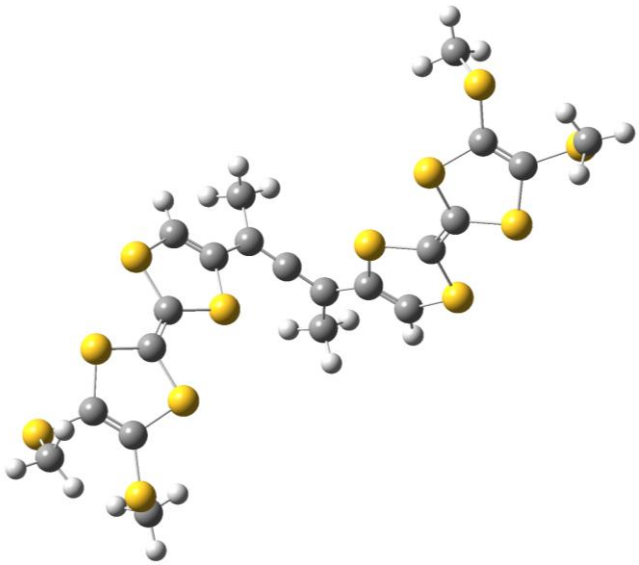


Figure S4. The optimized structure of compound **2.**

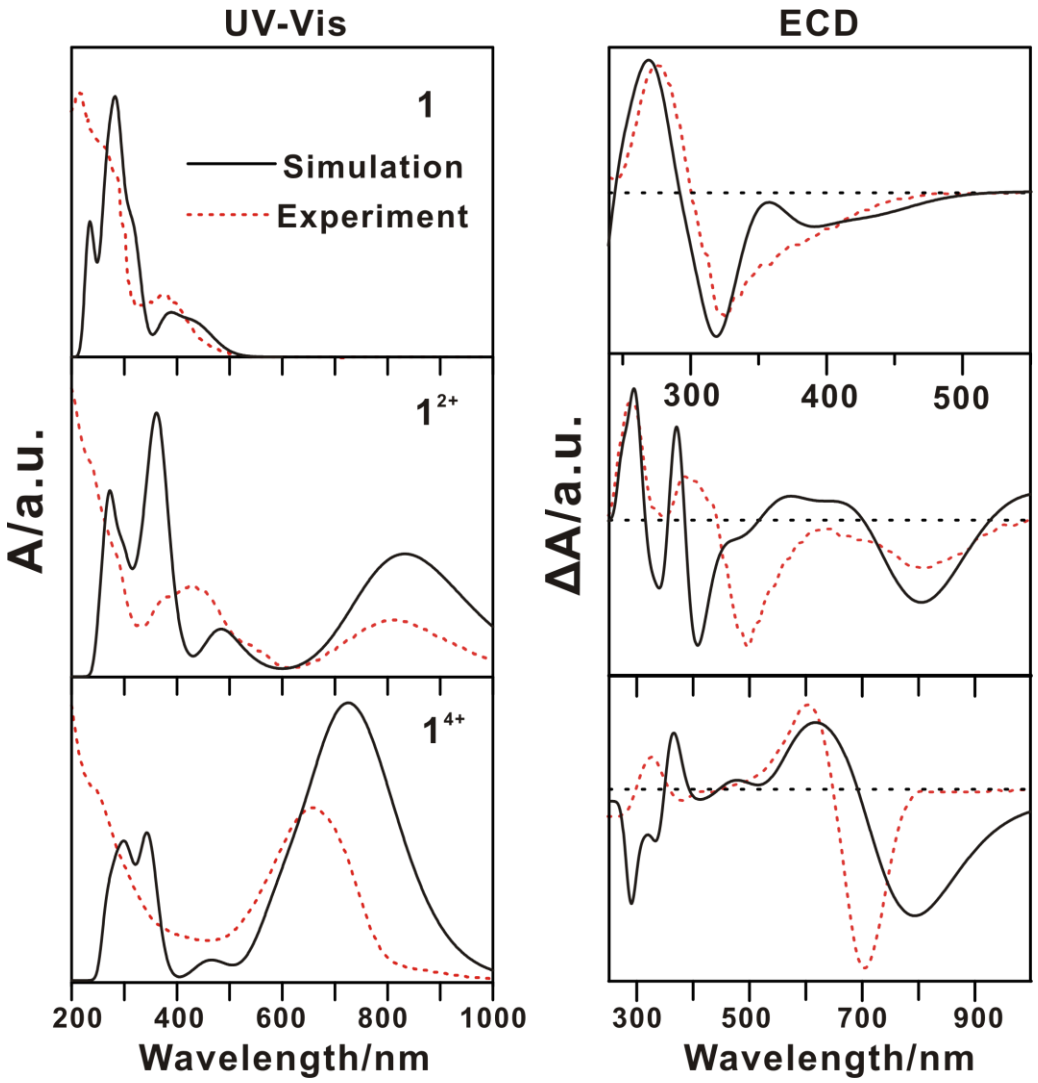


Figure S5. Calculated UV-Vis (left) and ECD (right) spectra in solution phases of **1**, $\mathbf{1}^{2+}$, and $\mathbf{1}^{4+}$ at the TDB3LYP/6-311++G(2d,2p) level of theory along with experimental UV-Vis and ECD (red dash line). Data to prepare the experimental ECD spectra were taken from ref 17.

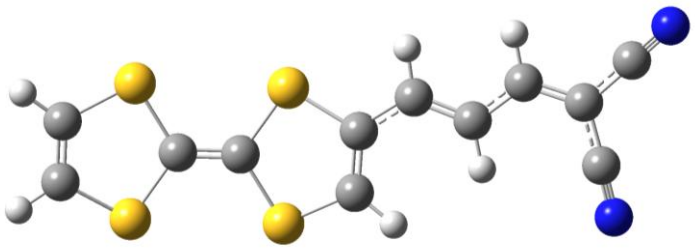


Figure S6. The optimized molecular geometry of the reference compound.

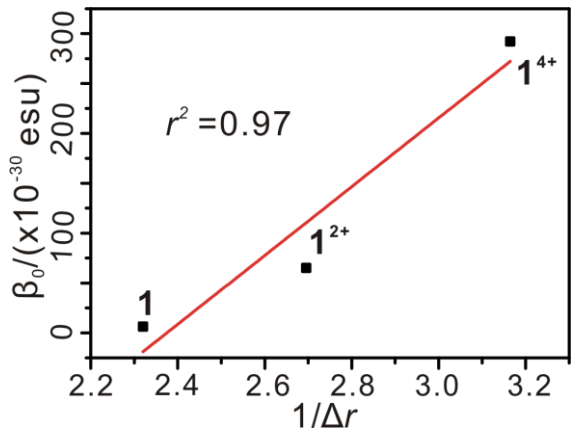


Figure. S7 Dependence of the first hyperpolarizability on the inverse of the BLA value (Δr).

Table S6. Cartesian Coordinates of **1** (B3LYP/6-31G**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	0.000000	0.000000	2.021863
2	6	0	-1.127505	0.681034	2.053392
3	6	0	1.127505	-0.681034	2.053392
4	6	0	2.221424	-0.262468	2.993677
5	6	0	2.777747	1.018214	2.909586
6	6	0	2.676473	-1.139704	3.986508
7	6	0	3.774970	1.413074	3.799455
8	1	0	2.428442	1.701514	2.144276
9	6	0	3.670436	-0.740888	4.87697
10	1	0	2.240290	-2.128701	4.069107
11	6	0	4.224497	0.535505	4.784172
12	1	0	4.201037	2.407033	3.720876
13	1	0	4.007785	-1.425735	5.646986
14	1	0	4.999455	0.843912	5.476798
15	6	0	-2.221424	0.262468	2.993677
16	6	0	-2.777747	-1.018214	2.909586
17	6	0	-2.676473	1.139704	3.986508
18	6	0	-3.774970	-1.413074	3.799455
19	1	0	-2.428442	-1.701514	2.144276
20	6	0	-3.670436	0.740888	4.87697
21	1	0	-2.240290	2.128701	4.069107

22	6	0	-4.224497	-0.535505	4.784172
23	1	0	-4.201037	-2.407033	3.720876
24	1	0	-4.007785	1.425735	5.646986
25	1	0	-4.999455	-0.843912	5.476798
26	6	0	-2.516562	2.489478	1.002894
27	1	0	-3.433087	2.237172	1.517091
28	6	0	-0.848504	3.809050	-0.48927
29	6	0	2.516562	-2.489478	1.002894
30	6	0	0.848504	-3.809050	-0.48927
31	1	0	3.433087	-2.237172	1.517091
32	6	0	1.353435	-1.835544	1.171412
33	6	0	-1.353435	1.835544	1.171412
34	16	0	-2.600251	3.797334	-0.15915
35	16	0	0.000000	2.376703	0.140016
36	16	0	0.000000	-2.376703	0.140016
37	16	0	2.600251	-3.797334	-0.15915
38	6	0	-1.586445	-6.573266	-1.81035
39	6	0	-0.406236	-7.209211	-1.97508
40	6	0	0.406236	7.209211	-1.97508
41	6	0	1.586445	6.573266	-1.81035
42	16	0	1.512637	4.812289	-1.52129
43	16	0	-1.066584	6.222101	-1.83026
44	16	0	1.066584	-6.222101	-1.83026
45	16	0	-1.512637	-4.812289	-1.52129
46	6	0	-0.230607	4.795902	-1.16574
47	6	0	0.230607	-4.795902	-1.16574
48	16	0	-0.131735	-8.927392	-2.31816
49	16	0	-3.189516	-7.294743	-1.99305
50	16	0	3.189516	7.294743	-1.99305
51	16	0	0.131735	8.927392	-2.31816
52	6	0	0.768104	9.078761	-4.03303
53	1	0	1.850508	8.966290	-4.05414
54	1	0	0.287269	8.347578	-4.68135
55	1	0	0.497729	10.084395	-4.35871
56	6	0	3.767725	7.311515	-0.24983
57	1	0	3.143026	7.974382	0.347171
58	1	0	3.767786	6.304801	0.165503
59	1	0	4.788867	7.693826	-0.27749
60	6	0	-0.768104	-9.078761	-4.03303
61	1	0	-1.850508	-8.966290	-4.05414
62	1	0	-0.287269	-8.347578	-4.68135
63	1	0	-0.497729	10.084395	-4.35871
64	6	0	-3.767725	-7.311515	-0.24983
65	1	0	-3.143026	-7.974382	0.347171

66	1	0	-3.767786	-6.304801	0.165503
67	1	0	-4.788867	-7.693826	-0.27749

Table S7. Cartesian Coordinates of $\mathbf{1}^{2+}$ (B3LYP/6-31G**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	y	z
1	6	0	0.000278	-0.000002	2.505440
2	6	0	-1.119562	0.700675	2.580214
3	6	0	1.120164	-0.700634	2.579816
4	6	0	2.197281	-0.279771	3.540777
5	6	0	2.783347	0.989428	3.443990
6	6	0	2.596246	-1.148058	4.569998
7	6	0	3.759232	1.382853	4.359026
8	1	0	2.480056	1.662078	2.647708
9	6	0	3.571510	-0.749098	5.482778
10	1	0	2.128866	-2.123230	4.669139
11	6	0	4.155313	0.515324	5.378310
12	1	0	4.212266	2.365599	4.275020
13	1	0	3.867638	-1.421929	6.281165
14	1	0	4.913761	0.823528	6.090645
15	6	0	-2.196204	0.280125	3.541817
16	6	0	-2.781677	-0.989448	3.446248
17	6	0	-2.595283	1.149033	4.570472
18	6	0	-3.757077	-1.382623	4.361902
19	1	0	-2.478304	-1.662584	2.650409
20	6	0	-3.570060	0.750322	5.483879
21	1	0	-2.128355	2.124512	4.668709
22	6	0	-4.153273	-0.514471	5.380614
23	1	0	-4.209652	-2.365659	4.278819
24	1	0	-3.866264	1.423648	6.281820
25	1	0	-4.911349	-0.822472	6.093433
26	6	0	-2.527785	2.565613	1.654953
27	1	0	-3.437712	2.260971	2.157007
28	6	0	-0.919194	3.963436	0.192546
29	6	0	2.527805	-2.566229	1.654990
30	6	0	0.918749	-3.963837	0.192885
31	1	0	3.437823	-2.261796	2.157006
32	6	0	1.346325	-1.905404	1.763692
33	6	0	-1.346073	1.905226	1.763844
34	16	0	-2.599487	3.999391	0.688043
35	16	0	-0.010072	2.603912	0.832544
36	16	0	0.010109	-2.603799	0.832473
37	16	0	2.599025	-4.000256	0.688406

38	6	0	-1.299604	-6.439697	-1.991510
39	6	0	-0.076879	-7.060959	-2.092965
40	6	0	0.075336	7.060288	-2.094149
41	6	0	1.298311	6.439559	-1.992417
42	16	0	1.336019	4.935629	-1.074504
43	16	0	-1.265205	6.276092	-1.279549
44	16	0	1.263915	-6.277103	-1.278450
45	16	0	-1.336776	-4.935507	-1.074005
46	6	0	-0.363213	4.938086	-0.623259
47	6	0	0.362426	-4.938518	-0.622649
48	16	0	0.233727	-8.613939	-2.875399
49	16	0	-2.744401	-7.118008	-2.713841
50	16	0	2.742889	7.118243	-2.714827
51	16	0	-0.235889	8.612924	-2.877013
52	6	0	-0.388922	8.122829	-4.647632
53	1	0	0.530791	7.662197	-5.008002
54	1	0	-1.245798	7.464531	-4.792527
55	1	0	-0.556993	9.060635	-5.181298
56	6	0	4.038367	5.905431	-2.276855
57	1	0	4.170764	5.837392	-1.195042
58	1	0	3.838299	4.926127	-2.716608
59	1	0	4.952013	6.309205	-2.717301
60	6	0	0.387498	-8.124272	-4.646073
61	1	0	-0.531867	-7.663185	-5.006751
62	1	0	1.244785	-7.466489	-4.790876
63	1	0	0.555168	-9.062268	-5.179531
64	6	0	-4.039368	-5.904410	-2.276521
65	1	0	-4.171823	-5.835817	-1.194750
66	1	0	-3.838820	-4.925396	-2.716701
67	1	0	-4.953163	-6.307975	-2.716849

Table S8. Cartesian Coordinates of $\mathbf{1}^{4+}$ (B3LYP/6-31G**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	y	z
1	6	0	0.000088	-0.000346	1.621397
2	6	0	-1.043849	0.801341	1.765651
3	6	0	1.043857	-0.802291	1.765526
4	6	0	2.126187	-0.378598	2.728829
5	6	0	3.060537	0.599469	2.356940
6	6	0	2.197849	-0.972562	3.999714
7	6	0	4.066140	0.973425	3.250022
8	1	0	3.013383	1.046988	1.367768
9	6	0	3.199952	-0.585877	4.888646

10	1	0	1.467935	-1.719897	4.296371
11	6	0	4.134691	0.384301	4.514861
12	1	0	4.798014	1.719994	2.959159
13	1	0	3.251052	-1.039808	5.872910
14	1	0	4.915522	0.678460	5.208573
15	6	0	-2.126767	0.376474	2.727818
16	6	0	-3.061914	-0.599928	2.353558
17	6	0	-2.198239	0.967812	3.999923
18	6	0	-4.068156	-0.974801	3.245539
19	1	0	-3.014845	-1.045450	1.363478
20	6	0	-3.200998	0.580211	4.887727
21	1	0	-1.467727	1.713856	4.298352
22	6	0	-4.136551	-0.388267	4.511594
23	1	0	-4.800643	-1.720066	2.952876
24	1	0	-3.251982	1.032123	5.872926
25	1	0	-4.917889	-0.683136	5.204434
26	6	0	-2.447284	2.734941	1.026929
27	1	0	-3.373730	2.317311	1.405772
28	6	0	-0.829810	4.422865	-0.045074
29	6	0	2.447578	-2.735022	1.025011
30	6	0	0.830342	-4.422041	-0.048786
31	1	0	3.373950	-2.317695	1.404370
32	6	0	1.238250	-2.100155	1.095641
33	6	0	-1.238018	2.099894	1.097052
34	16	0	-2.515779	4.301849	0.327768
35	16	0	0.099067	3.026361	0.408847
36	16	0	-0.098688	-3.026047	0.406390
37	16	0	2.516285	-4.301215	0.324271
38	6	0	-1.279035	-7.547988	-1.401108
39	6	0	0.043093	-7.976405	-1.696855
40	6	0	-0.042262	7.978660	-1.689898
41	6	0	1.279821	7.549976	-1.394324
42	16	0	1.406987	5.959815	-0.694580
43	16	0	-1.272204	6.792342	-1.394146
44	16	0	1.272990	-6.790348	-1.399846
45	16	0	-1.406325	-5.958434	-0.700017
46	6	0	-0.286761	5.588046	-0.647999
47	6	0	0.287417	-5.586705	-0.652808
48	16	0	0.679239	-9.521197	-2.179966
49	16	0	-2.650579	-8.569823	-1.636677
50	16	0	2.651396	8.572032	-1.628725
51	16	0	-0.678336	9.523889	-2.171705
52	6	0	0.447987	10.235025	-3.444617
53	1	0	1.307338	10.723228	-2.987594

54	1	0	0.736358	9.479325	-4.175170
55	1	0	-0.181706	10.986584	-3.928203
56	6	0	4.045739	7.627251	-0.924936
57	1	0	3.892379	7.444658	0.141428
58	1	0	4.213521	6.703561	-1.484282
59	1	0	4.910675	8.282027	-1.054737
60	6	0	-0.446998	10.231252	-3.453556
61	1	0	-1.306380	10.719844	-2.997008
62	1	0	-0.735320	-9.474931	-4.183485
63	1	0	0.182730	10.982398	-3.937737
64	6	0	-4.045037	-7.625685	-0.932253
65	1	0	-3.891949	-7.444236	0.134346
66	1	0	-4.212600	-6.701388	-1.490661
67	1	0	-4.909987	-8.280259	-1.062978

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